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Supporting Information for

Polyamorphic Transformations in Fe-Ni-C Liquids: Implications for Chemical Evolution of Terrestrial Planets

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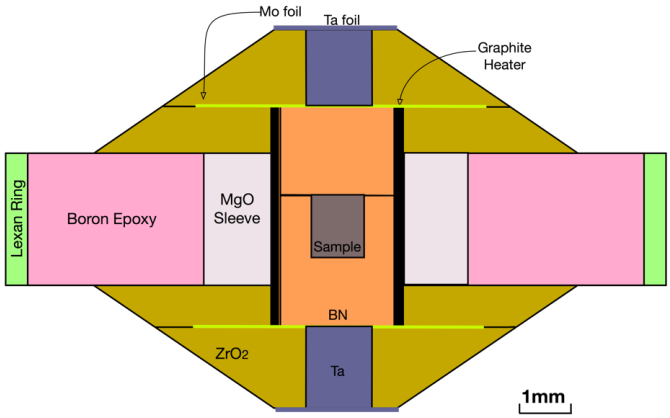

Figure S1. Cross-section of the cell assembly for liquid structure measurements in a Paris-Edinburgh Cell, modified after (Kono et al., 2014). The Fe-Ni-C sample is encapsulated in a boron nitride (BN) sample chamber.

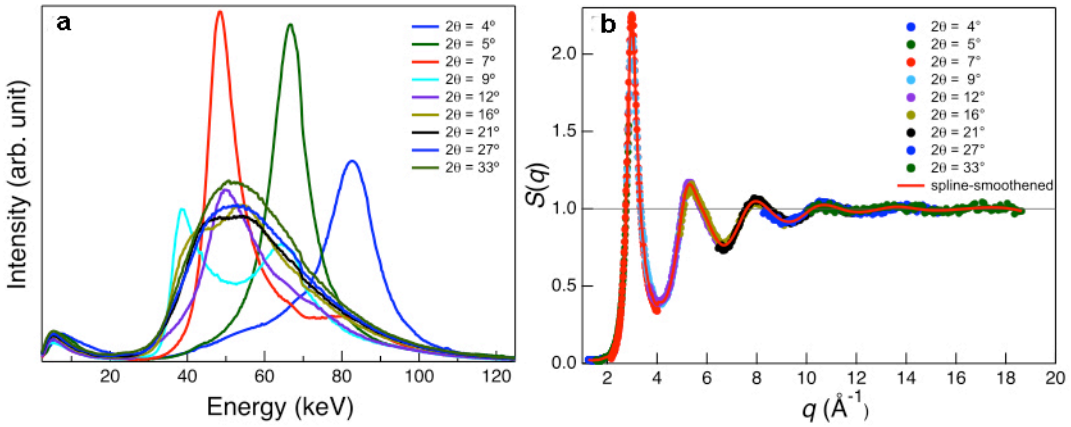

Figure S2. Representative experimental data and total structure factor *S*(*q*) of $Fe_{90}Ni_{10}$-5wt.% C liquid at 1.5 GPa and 1523 K. (a) Energy dispersive X-ray diffraction spectra of $Fe_{90}Ni_{10}$-5wt.% C liquid collected at 2θ angles from 4° to 33°. **(b)** Total structure factor *S*(*q*) of the $Fe_{90}Ni_{10}$-5wt.% C liquid at 1.5 GPa and 1523 K composed of structure factor fragments from measurements at different 2*θ* angles. The red solid curve is obtained after error-weighted spline-smoothing of the overlapped structure factor fragments.

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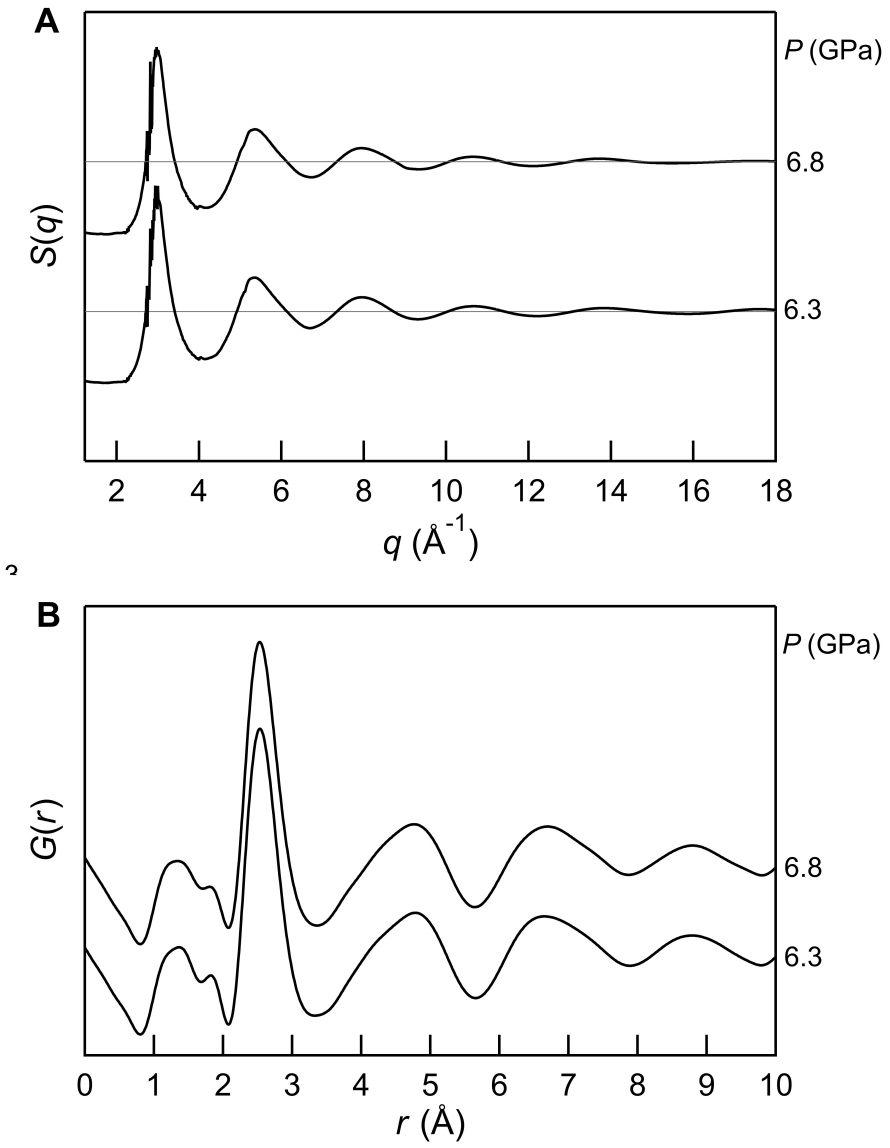

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36 **Figure S3. Additional results for the total structure factor *S*(*q*) and the reduced pair**
37 **distribution function *G*(*r*) of $Fe_{90}Ni_{10}$-5wt.%C liquids at high pressures and temperatures.**
38 **(a)** *S*(*q*), and **(b)** *G*(*r*) of $Fe_{90}Ni_{10}$-5wt.%C liquids at 6.3 and 6.8 GPa.
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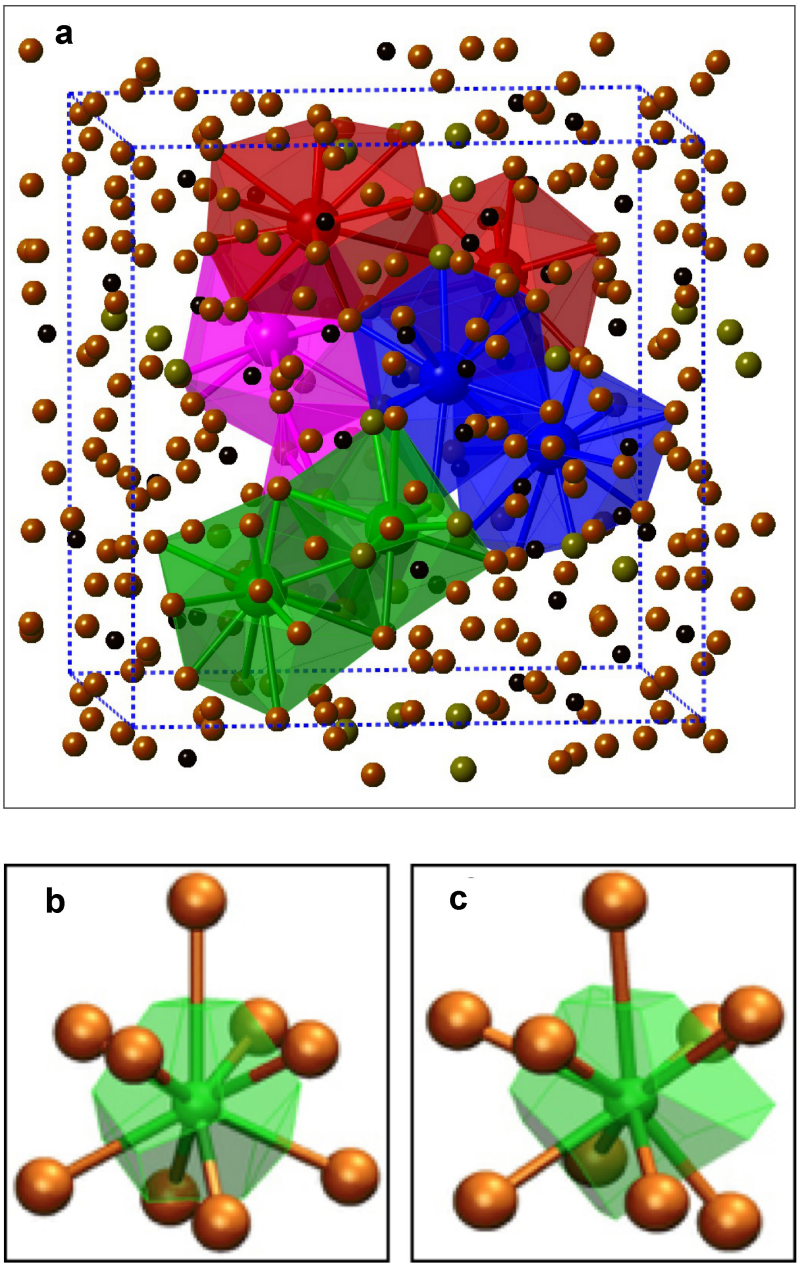

Figure S4. Structure information of Fe91Ni9-5wt.% C liquid and Fe3C from first-principles molecular dynamics simulations. (A) Snapshot of MD simulations with the computational super cell highlighted in dashed lines. The highlighted polyhedra are 1-atom corner-shared (red), 2-atom edge-shared (blue), 3-atom face-shared (magenta), and 4-atom distorted face-shared (green) connections of Fe/Ni – Fe/Ni pair with their second nearest neighbors. Center atoms in the polyhedra are Fe/Ni atoms, with their sizes enlarged for clarity. Fe: brown, Ni: olive, C: black. (B) Carbon coordination environment of crystalline Fe3C. (C) Carbon coordination environment of Fe91Ni9-5wt.% C liquid at 5.1 GPa, 1673 K, the center atoms are carbon. In B, C, green polyhedral are the Voronoi polyhedral of the center carbon.